Relativistic quantum mechanics

The theory of quantum mechanics that we have studied thus far is based on the nonrelativistic definition of energy

$$E = \frac{p^2}{2m} + V$$

The replacement of p, V, and E with the appropriate operators leads to the Schrödinger equation. However, special relativity, indicates that the equation above is only an approximation, which is valid at low velocities $\left(\frac{v}{c} << 1\right)$. When particle velocity becomes comparable to the speed of light, this equation breaks down.

Klein - Gordon equation

In special relativity the equation that gives the correct relation between p and E at any velocity (or momentum) is

$$E^2 = p^2c^2 + m^2c^4$$

Here we assume $V=0$ for simplicity. In the limit $v<<c$ the above equation reduces to

$$E = \frac{p^2}{2m} + mc^2$$

The term mc^2 in special relativity is called the rest energy of the particle. Nonrelativistic quantum mechanics ignores this rest energy, but it is included in the equations of relativistic quantum mec

In order to derive an equation for the wave function that corresponds to $E^2 = p^2c^2 + m^2c^4$, let us follow a procedure that is very similar to the "derivation" of the Schrödinger equation.

Assume that we have $\phi(\vec{r},t)$ that is an eigenfunction of the energy operator $i\hbar\frac{\partial}{\partial t}$ with eigenvalue E, and also an eigenfunction of the momentum operator $-i\hbar\nabla$ with eigenvalue $\vec{p}$. Then

$$\left(i\hbar\frac{\partial}{\partial t}\right)^2\phi = E^2\phi$$

and

$$(-i\hbar\nabla)^2\phi = p^2\phi$$

we can reproduce $E^2 = p^2c^2 + m^2c^4$ by writing

$$\left(i\hbar\frac{\partial}{\partial t}\right)^2\phi = (-i\hbar\nabla)^2c^2\phi + m^2c^4\phi$$

If we now make an assumption that the last equation is always valid, regardless of whether or not ϕ is an eigenfunction of energy or momentum, after simplification we get

$$\frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} - \nabla^2\phi + \frac{m^2c^2}{\hbar^2}\phi = 0$$

This equation is called the Klein-Gordon equation. The Klein-Gordon equation describes particles with spin 0. Further, this equation leads to some problems connected with the interpretation of probabilities.

For the Schrödinger equation the probability density is given by $|\psi|^2$. But it is not true that the corresponding quanlity for the KG equation is $|\phi|^2$

In analogy with a classical fluid with density ρ and velocity $\vec{v}$, the rate $\frac{\partial \rho}{\partial t}$ at which the density changes at a fixed point is given by

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \qquad \text{(continuity equation)}$$

or after using the divergence theorem

$$\int_V \frac{\partial \rho}{\partial t} + \int_V \nabla \cdot (\rho \vec{v})\, dV = 0$$

$$\int_V \frac{\partial \rho}{\partial t} + \int_S (\rho \vec{v}) \cdot d\vec{S} = 0$$

In quatum mechanics, probability can be treated in exactly the same way. The quantity equivalent to the density ρ is just the probability density. We can define a probability current $\vec{J}$ that satisfies the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0$$

In nonrelativistic QM

Substituting $\rho = \psi^* \psi$ into the above equation yields

$$\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} + \nabla \cdot \vec{J} = 0 \qquad (*)$$

but

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi$$

Multiplying by $\frac{-i\psi^*}{\hbar}$ gives $\quad \psi^* \frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \psi^* \nabla^2 \psi$

The complex conjugate gives $\quad \psi \frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m} \psi \nabla^2 \psi^*$

Substituting this into equation (*) gives

$$\nabla \cdot \vec{J} = \frac{i\hbar}{2m}\left(\psi \nabla^2 \psi^* - \psi^* \nabla^2 \psi\right)$$

which can be integrated to give the expression for $\vec{J}$:

$$\vec{J} = \frac{i\hbar}{2m}\left(\psi \nabla \psi^* - \psi^* \nabla \psi\right).$$

Now taking the same expression for $\vec{J}$, but using the KG equation instead of the SE, we can derive an expression for ρ that satisfies the continuity equation

$$\rho = \frac{i\hbar}{2mc^2}\left(\phi^* \frac{\partial \phi}{\partial t} - \phi \frac{\partial \phi^*}{\partial t}\right)$$

The latter expression for ρ can be negative.

Further, by using $E^2 = p^2c^2 + m^2c^4$ we have inadvertedly introduced negative energy solutions

$$E = \sqrt{p^2c^2 + m^2c^4} \,. \qquad E = -\sqrt{p^2c^2 + m^2c^4}$$

Let us consider the solution to the KG equation for a particle at rest

$$\vec{p} = 0 \quad \Rightarrow \quad -i\hbar \nabla \phi = 0 \quad \Rightarrow \quad \frac{1}{c^2}\frac{\partial^2 \phi}{\partial t^2} + \frac{m^2c^2}{\hbar^2}\phi = 0$$

$$\phi = A_1 e^{\frac{imc^2 t}{\hbar}} + A_2 e^{-\frac{imc^2 t}{\hbar}} \qquad (A_{1,2} = \text{const})$$

By applying the energy operator $i\hbar\frac{\partial}{\partial t}$ to each term in the last expression we see that the first one corresponds to the negative energy $E = -mc^2$, while the second term corresponds to the state with positive energy $E = mc^2$

Because the KG equation contains a second derivative with respect to t, two boundary conditions are necessary to determine the two unknown constants.

Dirac equation

Let us consider what happens if we try to construct an operator equation corresponding to $E^2 = p^2c^2 + m^2c^4$ but restrict the equation to be the first order in all of the operators. We could write

$$i\hbar \frac{\partial \psi}{\partial t} = \left[-i\hbar c \left(\alpha_1 \frac{\partial}{\partial x} + \alpha_2 \frac{\partial}{\partial y} + \alpha_3 \frac{\partial}{\partial z} \right) + \beta m c^2 \right] \psi$$

where $\alpha_1, \alpha_2, \alpha_3$, and β are constants to be determined. In order to find the values of these constants, we square the operator on both sides, and require the final result to reduce to the Klein-Gordon equation.

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = \left(-i\hbar c \sum_{j=1}^{3} \alpha_j \nabla_j + \beta m c^2 \right) \left(-i\hbar c \sum_{k=1}^{3} \alpha_k \nabla_k + \beta m c^2 \right) \psi$$

$$= \left(-\hbar^2 c^2 \sum_{j=1}^{3} \sum_{k=1}^{3} \alpha_j \alpha_k \nabla_j \nabla_k - i\hbar m c^3 \sum_{j} (\beta \alpha_j + \alpha_j \beta) \nabla_j + \beta^2 m^2 c^4 \right) \psi$$

where $\nabla_1 = \frac{\partial}{\partial x}$ $\nabla_2 = \frac{\partial}{\partial y}$ $\nabla_3 = \frac{\partial}{\partial z}$. We want to reduce to the KG equation, which can be written as

$$-\hbar^2 \frac{\partial^2 \phi}{\partial t^2} = -\hbar^2 c^2 \nabla^2 \phi + m^2 c^4 \phi$$

In order for our equation to reduce to the KG equation, the first term on the right-hand side must simplify to $-\hbar^2 c^2 \vec{\nabla}^2 \psi$. That requires $\alpha_j \alpha_j = 1$

and $\alpha_j\alpha_k + \alpha_k\alpha_j = 0 \qquad j \neq k$

The second term on the right hand side of our equation must vanish, which gives

$$\beta\alpha_j + \alpha_j\beta = 0$$

Finally, the last term on the right-hand side of equation must reduce to m^2c^4, so that $\beta^2 = 1$.

To summarize:

$$\alpha_1^2 = \alpha_2^2 = \alpha_3^2 = \beta^2 = 1$$

but the four constants all anticommute with each other ($\alpha_i\alpha_j = -\alpha_j\alpha_i \quad i \neq j$). It turs out to be impossible to find four numbers that satisfy these relations. It becomes possible if we take $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ and β to be matrices. For example, the Pauli matrices satisfy exactly the desired relations: $\sigma_i^2 = I$ and $\sigma_i\sigma_j + \sigma_j\sigma_i = 0 \ (i \neq j)$. The problem is that there are only three of these matrices while we need four. It turns out the minimum size of the matrices must be 4×4. If we have matrices that means that the wave function in our equation is no longer a one-component object (as in the KG or Schrödinger equations). It is a four-component vector-column (called bispinor). There are an infinite number of different choices for 4×4 matrices that satisfy the necessary relations. This choice does not change any observables. The conventional choice is

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

With these values for α_i and β we can go back to our original equation and write

$$i\hbar \frac{\partial \psi}{\partial t} = -i\hbar c(\vec{\alpha}\cdot\nabla)\psi + \beta m c^2 \psi \quad \leftarrow \text{Dirac equation}$$

where $\vec{\alpha}\cdot\nabla \equiv \alpha_1 \frac{\partial}{\partial x} + \alpha_2 \frac{\partial}{\partial y} + \alpha_3 \frac{\partial}{\partial z}$

As mentioned above

$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$ is a four-component object, where each component is a function of position and time

Let us now consider the probability density and current. The adjoint of DE is

$$-i\hbar \frac{\partial \psi^\dagger}{\partial t} = i\hbar c(\nabla\psi^\dagger)\cdot\vec{\alpha} + \psi^\dagger \beta m c^2 \qquad (\alpha_j \text{ and } \beta \text{ are Hermitian})$$

Using DE and adjont of DE, as well as the time derivatives of ψ and $\psi^\dagger$:

$$\frac{\partial}{\partial t}(\psi^\dagger\psi) = \psi^\dagger \frac{\partial \psi}{\partial t} + \frac{\partial \psi^\dagger}{\partial t}\psi = -c\vec{\nabla}\cdot(\psi^\dagger \vec{\alpha}\psi)$$

This equation looks just like the continuity equation if we take

$$\rho = \psi^\dagger\psi \qquad J = c\psi^\dagger\vec{\alpha}\psi$$

Note that the Dirac probability density is always positive:

$$\rho = \psi^{+}\psi = |\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2 + |\psi_4|^2$$

Now let us consider the solutions of the DE for a particle at rest.

$$\vec{p} = 0 \implies -i\hbar c(\vec{\alpha}\cdot\vec{\nabla})\psi = 0$$

Then

$$i\hbar \frac{\partial\psi}{\partial t} = \beta m c^2 \psi$$

or, in components

$$i\hbar \frac{\partial\psi_1}{\partial t} = mc^2\psi_1$$

$$i\hbar \frac{\partial\psi_2}{\partial t} = mc^2\psi_2$$

$$i\hbar \frac{\partial\psi_3}{\partial t} = -mc^2\psi_3$$

$$i\hbar \frac{\partial\psi_4}{\partial t} = -mc^2\psi_4$$

Solving for $\psi_1, \psi_2, \psi_3, \psi_4$ and recombining them into a vector-column gives four independent solutions

The first two of them are:

$$\begin{pmatrix}1\\0\\0\\0\end{pmatrix} e^{-\frac{imc^2t}{\hbar}} \qquad \begin{pmatrix}0\\1\\0\\0\end{pmatrix} e^{-\frac{imc^2t}{\hbar}}$$

The energies corresponding to these two solutions can be determined by applying the energy operator $i\hbar\frac{\partial}{\partial t}$:

$$E = mc^2 \quad \text{for both}$$

This is precisely the expected result for the energy of the particle at rest

But why there are two linearly-independent solutions corresponding to the same energy (rest energy)
These solutions describe a two-component object – spinor
Thus, the Dirac equation naturally describes a particle with spin 1/2, while ψ combines both the spatial and spin information into a single object – spinor.

$\psi = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} e^{-\frac{imc^2 t}{\hbar}}$ describes a particle at rest with $m_s = +\frac{1}{2}$, while

$\psi = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} e^{-\frac{imc^2 t}{\hbar}}$ describes a particle at rest with $m_s = -\frac{1}{2}$

Combined into a linear combination these two solutions can describe any spin state of a spin 1/2 particle.

The other two solutions (#3 and #4) are

$$\psi = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} e^{\frac{imc^2 t}{\hbar}} \quad \text{and} \quad \psi = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} e^{\frac{imc^2 t}{\hbar}}$$

$E = -mc^2$

correspond to a negative energy! They are interpreted as anti-particle solutions
The holes in the see of negative-energy states are called antiparticles